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Sequences, modular forms and cellular integrals

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Abstract

It is well-known that the Apéry sequences which arise in the irrationality proofs for $\zeta(2)$ and $\zeta(3)$ satisfy many intriguing arithmetic properties and are related to the pth Fourier coefficients of modular forms. In this paper, we prove that the connection to modular forms persists for sequences associated to Brown's cellular integrals and state a general conjecture concerning supercongruences.

1. *Introduction*

Period integrals on the moduli space $\mathcal{M}_{0,N}$ of curves of genus 0 with N marked points have featured prominently in a variety of mathematical and physical contexts. These period integrals are of particular importance as, for example, it is now known that they are $\mathbb{Q}$-linear combinations of multiple zeta values [**12**] thereby proving a conjecture of Goncharov and Manin [**22**], provide an effective computation of a large class of Feynman integrals [**10**], occur in superstring theory [**11**], [**41**] and have potential connections to higher Frobenius limits in relation to the Gamma conjecture [**21**]. Recently, Brown [**13**] introduced a program where such period integrals play a central role in understanding irrationality proofs of values of the Riemann zeta function. Before discussing this program, we first briefly review the classical situation and some subsequent developments.

Inspired by Apéry, Beukers [**7**] gave another proof of the irrationality of $\zeta(2)$ and $\zeta(3)$ by considering the integrals

$$I_n := (-1)^n \int_0^1 \int_0^1 \frac{x^n(1-x)^n y^n(1-y)^n}{(1-xy)^{n+1}}\, dxdy \tag{1·1}$$

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and

$$J_n := \frac{1}{2}\int_0^1\int_0^1\int_0^1 \frac{x^n(1-x)^n y^n(1-y)^n w^n(1-w)^n}{(1-(1-xy)w)^{n+1}}\,dxdydw. \tag{1·2}$$

He showed that

$$I_n = a(n)\zeta(2) + \tilde{a}(n) \qquad \text{and} \qquad J_n = b(n)\zeta(3) + \tilde{b}(n),$$

where $\tilde{a}(n)$ and $\tilde{b}(n)$ are explicit rational numbers and

$$a(n) = \sum_{k=0}^{n}\binom{n}{k}^2\binom{n+k}{k}, \qquad b(n) = \sum_{k=0}^{n}\binom{n}{k}^2\binom{n+k}{k}^2 \tag{1·3}$$

are the *Apéry numbers*. Since their introduction, there has been substantial interest in both the intrinsic arithmetic properties of the Apéry numbers and their relationship to modular forms. For example, consider

$$\eta^6(4z) =: \sum_{n=1}^{\infty}\alpha(n)q^n,$$

the unique newform in $S_3(\Gamma_0(16), (\frac{-4}{\cdot}))$, where $\eta(z) = q^{1/24}\prod_{n\geqslant 1}(1-q^n)$ is the Dedekind eta-function, $q = e^{2\pi iz}$ and $z \in \mathbb{H}$. Ahlgren [**1**] showed that, for all primes $p \geqslant 5$,

$$a\Big(\frac{p-1}{2}\Big) \equiv \alpha(p) \pmod{p^2}, \tag{1·4}$$

thus confirming a conjecture in [**42**]. In [**3**], Ahlgren and Ono proved a conjecture of Beukers [**9**] which stated that, if p is an odd prime, then

$$b\Big(\frac{p-1}{2}\Big) \equiv \beta(p) \pmod{p^2}, \tag{1·5}$$

where

$$\eta^4(2z)\eta^4(4z) =: \sum_{n=1}^{\infty}\beta(n)q^n$$

is the unique newform in $S_4(\Gamma_0(8))$. Both of these influential results required the existence of an underlying modular Calabi–Yau variety, specifically a $K3$-surface for (1·4) and a Calabi–Yau 3-fold for (1·5) in order to relate the pth Fourier coefficients to finite field hypergeometric series. Concerning arithmetic properties, Coster [**17**] proved the supercongruences

$$a(mp^r) \equiv a(mp^{r-1}) \pmod{p^{3r}} \tag{1·6}$$

and

$$b(mp^r) \equiv b(mp^{r-1}) \pmod{p^{3r}} \tag{1·7}$$

for primes $p \geqslant 5$ and integers $m, r \geqslant 1$. Other supercongruences of this type have been studied in numerous works (for example, see [**4**], [**8**], [**15**], [**16**], [**20**], [**25**], [**31**]–[**34**], [**43**]). In order to view (1·4)–(1·7) from a general perspective, we discuss the setup from [**13**].

Recall that $\mathcal{M}_{0,N}$, $N \geqslant 4$, is the moduli space of genus zero curves (Riemann spheres) with N ordered marked points $(z_1, \ldots, z_N)$. It is the set of N-tuples of distinct points $(z_1, \ldots, z_N)$ modulo the equivalence relation given by the action of PSL_2. This action is triply-transitive and so there is a unique representative of each equivalence class such that

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$z_1 = 0$, $z_{N-1} = 1$ and $z_N = \infty$. We introduce simplicial coordinates on $\mathcal{M}_{0,N}$ by setting $t_1 = z_2, t_2 = z_3, \ldots, t_{N-3} = z_{N-2}$. This yields the identification

$$\mathcal{M}_{0,N} \cong \{(t_1, \ldots, t_{N-3}) \in (\mathbb{P}^1 \setminus \{0, 1, \infty\})^{N-3} \mid t_i \neq t_j \text{ for all } i \neq j\}.$$

A typical period integral on $\mathcal{M}_{0,N}$ can be given as

$$\int_{S_N} \prod t_i^{a_i} (1 - t_j)^{b_j} (t_i - t_j)^{c_{ij}} dt_1 \ldots dt_{N-3}, \tag{1·8}$$

where a_i, b_j and $c_{ij} \in \mathbb{Z}$ are such that (1·8) converges and the simplex

$$S_N = \{(t_1, \ldots, t_{N-3}) \in \mathbb{R}^{N-3} : 0 < t_1 < \cdots < t_{N-3} < 1\}$$

is a connected component of $\mathcal{M}_{0,N}(\mathbb{R})$. It was proved by Brown [**12**] that the integrals (1·8) are $\mathbb{Q}$-linear combinations of multiple zeta values of weight up to and including $N - 3$. That these typically involve multiple zeta values of all weights is an obstruction to irrationality proofs. For example, generic period integrals on $\mathcal{M}_{0,6}$ yield linear forms in $1, \zeta(2)$ and $\zeta(3)$. To ensure the vanishing of coefficients, we consider a variant of the classical "dinner table problem" [**6**], [**38**].

Suppose we have $N \geqslant 5$ people sitting at a round table. We permute them such that each person has two new neighbours. We represent the new seating arrangement (non-uniquely) by a permutation $\sigma = \sigma_N$ on $\{1, 2, \ldots, N\}$ and write $\sigma = (\sigma(1), \ldots, \sigma(N))$. A permutation σ is called *convergent* if no set of k elements in $\{1, \ldots, N\}$ are simultaneously consecutive for $\{1, \ldots, N\}$ and σ for all $2 \leqslant k \leqslant N - 2$. If $N \leqslant 7$, then this is equivalent to the dinner table problem. For $N \geqslant 8$, this is a new condition. The main idea of [**13**] is to associate a rational function f_σ and a differential $(N - 3)$-form ω_σ to a given σ as follows. Formally, we define

$$f_\sigma = \prod_i \frac{z_i - z_{i+1}}{z_{\sigma(i)} - z_{\sigma(i+1)}} \qquad \text{and} \qquad \omega_\sigma = \frac{dt_1 \ldots dt_{N-3}}{\prod_i z_{\sigma(i)} - z_{\sigma(i+1)}}, \tag{1·9}$$

where the product is over all indices i modulo N, $z_1 = 0$ and $z_{N-1} = 1$. We remove factors with z_N and then let $z_{i+1} \mapsto t_i$ for $i = 1, 2, \ldots, N - 3$. If we consider the *cellular integral*

$$I_\sigma(n) = I_{N,\sigma}(n) := \int_{S_N} f_\sigma^n \, \omega_\sigma, \tag{1·10}$$

then $I_\sigma(n)$ converges if and only if σ is convergent. For $n = 0$, we then obtain the cell-zeta values $\zeta_\sigma(N - 3) = I_\sigma(0)$ studied in [**14**], which are multiple zeta values of weight $N - 3$. More generally, by [**13**, corollary 8·2], $I_\sigma(n)$ is a $\mathbb{Q}$-linear combination of multiple zeta values of weight less than or equal to $N - 3$. Suppose that this linear combination is of the form $A_{\sigma_N}(n)\zeta_\sigma(N - 3)$, with $A_{\sigma_N}(n) \in \mathbb{Q}$, plus a combination of multiple zeta values of weight less than $N - 3$ (note that $A_{\sigma_N}(n)$ is necessarily unique if multiple zeta values of different weight are linearly independent over $\mathbb{Q}$; alternatively, since this independence remains open, a unique value can be selected, unconditionally, by working motivically [**13**]). We then say that $A_\sigma(n) = A_{\sigma_N}(n)$ is the *leading coefficient* of the cellular integral $I_\sigma(n)$. By construction, $A_\sigma(0) = 1$. Conjecturally, we can define leading coefficients in this fashion for all convergent σ. Since we will be concerned with specific permutations σ, in which case the linear combinations of multiple zeta values can be made explicit, this issue will not disturb our discussion.

For example, if $N = 5$, then $\sigma_5 = (1, 3, 5, 2, 4)$ is the unique (up to dihedral symmetry, see Section 2) convergent permutation, $I_{\sigma_5}(n)$ recovers Beukers' integral (1·1) after a change

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of variables, and the leading coefficients $A_{\sigma_5}(n)$ are the Apéry numbers $a(n)$. Similarly, for $N = 6$, one obtains (1·2) upon considering $\sigma_6 = (1, 5, 3, 6, 2, 4)$ and the leading coefficients $A_{\sigma_6}(n)$ are the Apéry numbers $b(n)$.

This general framework raises some natural questions. Is there an analogue of (1·4) and (1·5) for $N \geqslant 7$? Do the leading coefficients $A_\sigma(n)$ satisfy supercongruences akin to (1·6)? The first main result generalises (1·4) to all odd weights greater than or equal to 3.

THEOREM 1·1. *For each odd positive integer $N \geqslant 5$, there exists a convergent σ_N and a modular form $f_k(z) =: \sum_{n=1}^{\infty} \gamma_k(n)q^n$ of weight $k = N - 2$ such that, for all primes $p \geqslant 5$,*

$$A_{\sigma_N}\left(\frac{p-1}{2}\right) \equiv \gamma_k(p) \pmod{p^2}. \tag{1·11}$$

As the product of cellular integrals is not necessarily a cellular integral (see Example 2·4), powers of the Apéry numbers $a(n)$ are not automatically leading coefficients. We prove Theorem 1·1 by carefully constructing an explicit family of convergent σ_N such that $A_{\sigma_N}(n) = a(n)^{(N-3)/2}$ and the required modular forms $f_k(z)$. For example, if $N = 5$, then $A_{\sigma_5}(n) = a(n)$ and $f_3(z) = \eta^6(4z)$. Thus, we recover (1·4). Now, consider the convergent permutation $\sigma_8 = (8, 3, 6, 1, 4, 7, 2, 5)$ and

$$\eta^{12}(2z) =: \sum_{n=1}^{\infty} \gamma(n)q^n,$$

the unique newform in $S_6(\Gamma_0(4))$. Our second main result is a higher weight version of (1·5).

THEOREM 1·2. *Let p be an odd prime. Then*

$$A_{\sigma_8}\left(\frac{p-1}{2}\right) \equiv \gamma(p) \pmod{p^2}. \tag{1·12}$$

In [**13**, section 10·1], Brown provided the following table for the number $\mathcal{C}_N$ of convergent σ_N (up to symmetries):

Table 1. *$\mathcal{C}_N$ for $5 \leqslant N \leqslant 11$*

N	5	6	7	8	9	10	11
$\mathcal{C}_N$	1	1	5	17	105	771	7028

Using the techniques from Section 3, we have obtained explicit binomial sum expressions for all 898 of the leading coefficients $A_{\sigma_N}(n)$ for $7 \leqslant N \leqslant 10$. For example, if $N = 7$, then the convergent permutations and associated leading coefficients are given in Table 2. The ordinary generating functions of these five sequences satisfy fourth order differential equations of Calabi–Yau type, and thus appear as sequences in the table [**5**] (where they are numbered as 193, 243, 101, 198 and 27). The remaining list of convergent permutations and binomial sum expressions for the leading coefficients are available upon request.

Based on numerical evidence, we make the following conjecture which suggests that (1·6) is a generic property of leading coefficients.

CONJECTURE 1·3. *For each $N \geqslant 5$ and convergent σ_N, the leading coefficients $A_{\sigma_N}(n)$ satisfy*

$$A_{\sigma_N}(mp^r) \equiv A_{\sigma_N}(mp^{r-1}) \pmod{p^{3r}} \tag{1·13}$$

for all primes $p \geqslant 5$ and integers m, $r \geqslant 1$.

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Table 2. *Convergent permutations σ_7 and leading coefficients $A_{\sigma_7}(n)$*

$(7, 2, 4, 1, 6, 3, 5)$	$\sum_{j,k=0}^{n} \binom{n}{k}^2 \binom{n}{j}^2 \binom{n+k+j}{n} \binom{k+j}{k}$
$(7, 2, 4, 6, 1, 3, 5)$	$\sum_{j,k=0}^{n} \binom{n}{k} \binom{n}{j} \binom{n+k}{n} \binom{n+j}{n} \binom{n+k+j}{n} \binom{n}{k-j}$
$(7, 2, 5, 1, 3, 6, 4)$	$\left[\sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{n}\right]^2$
$(7, 2, 5, 1, 4, 6, 3)$	$\sum_{j,k=0}^{n} \binom{n}{k}^2 \binom{n}{j}^2 \binom{n+k}{n} \binom{k+j}{n}$
$(7, 3, 6, 2, 5, 1, 4)$	$\sum_{j,k=0}^{n} \binom{n}{k}^2 \binom{n}{j}^2 \binom{n+k}{n} \binom{n-k+j}{n}$

Given Theorems 1·1 and 1·2, it is natural to wonder if such supercongruences hold for all leading coefficients $A_{\sigma_N}(n)$. Do they arise from L-series attached to Galois representations? It appears that a result similar to (1·5) and (1·12) also holds for a convergent σ_{10} and modular form of weight 8. This and other observations will be the subject of forthcoming work. Finally, it would be of interest to examine Theorems 1·1 and 1·2 and Conjecture 1·3 from the recent "motivic" perspective of [**40**].

The paper is organised as follows. In Section 2, we first discuss the necessary background on dihedral symmetries, the multiplicative structure of cellular integrals and modular forms with complex multiplication, then prove Theorem 1·1. In Section 3, we explain how to derive multiple binomial sum representations for the leading coefficients. In Section 4, we prove some preliminary results on combinatorial congruences, recall finite field hypergeometric series and then prove Theorem 1·2.

2. *Proof of Theorem* 1·1

2·1. *Dihedral symmetries and multiplicative structures*

Let Σ_N be the symmetric group on $\{1, 2, \ldots, N\}$. A *dihedral structure* on $\{1, 2, \ldots, N\}$ is an equivalence class of permutations $\sigma \in \Sigma_N$, where the equivalences are generated by

$$(\sigma_1, \sigma_2, \ldots, \sigma_N) \sim (\sigma_2, \sigma_3, \ldots, \sigma_N, \sigma_1)$$
$$(\sigma_1, \sigma_2, \ldots, \sigma_N) \sim (\sigma_N, \sigma_{N-1}, \ldots, \sigma_1).$$

A *configuration* on $\{1, 2, \ldots, N\}$ is an equivalence class $[\delta, \delta']$ of pairs (δ, δ') of dihedral structures modulo the equivalence relations

$$(\delta, \delta') \sim (\sigma\delta, \sigma\delta')$$

for $\sigma \in \Sigma_N$. Associated to every permutation $\sigma \in \Sigma_N$ is the configuration $[\sigma] := [\mathrm{id}, \sigma]$. Clearly, every configuration can be thus represented. Indeed, the configurations on $\{1, 2, \ldots, N\}$ can be identified with the double cosets $D_{2N} \backslash \Sigma_N / D_{2N}$, where D_{2N} are the dihedral permutations of Σ_N. Henceforth, we will not make a distinction between permutations and configurations. The *dual* of a configuration $[\delta, \delta']$ is the configuration $[\delta', \delta]$. Equivalently, the dual of $[\sigma]$ is $[\sigma]^\vee := [\sigma^{-1}]$. For further details, we refer to [**13**, section 3·1].

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The notion of a configuration is important for our considerations because, up to a possible factor of $(-1)^n$, the cellular integral $I_\sigma(n)$ only depends on the configuration $[\sigma]$.

In [**13**, section 6·2], Brown describes the following partial multiplication on pairs of dihedral structures. A pair of dihedral structures (δ, δ') on $\{1, 2, \dots, N\}$ is *multipliable* along the triple $t = (t_1, t_2, t_3)$, where $t_1, t_2, t_3 \in \{1, 2, \dots, N\}$ are distinct, if the elements t_1, t_2, t_3 are consecutive in δ and the elements t_1, t_3 are consecutive in δ'.

Let (α, α') and (β, β') be dihedral structures on $X = \{1, 2, \dots, N\}$ and $Y = \{1, 2, \dots, M\}$, respectively. If (α, α') is multipliable along s, and (β', β) (the dual of (β, β')) is multipliable along t, then the product

$$(\gamma, \gamma') := (\alpha, \alpha') \star_{s,t} (\beta, \beta')$$

is a pair of dihedral structures on the disjoint union Z of X and Y, where each of the three elements s_1, s_2, s_3 from X gets identified with the corresponding element t_1, t_2, t_3 from Y. The dihedral structure γ is the unique structure such that its restriction to X (respectively, Y) coincides with α (respectively, β). We say that γ was obtained by shuffling α and β (more general such shuffles are described in [**14**, section 2·3·1]). γ' is likewise obtained by shuffling α' and β'.

In order to work explicitly, we identify this disjoint union of X and Y with the set $Z = \{1, 2, \dots, M + N - 3\}$ in such a way that Y is the natural subset of Z, while the $N - 3$ elements $1, 2, \dots, N$ of X, with s_1, s_2, s_3 removed, are identified, in that order, with the elements $M + 1, M + 2, \dots, M + N - 3$ of Z. We note that different choices for this identification lead to the same configuration $[\gamma, \gamma']$.

Example 2·1. For illustration, let us multiply $(\alpha, \alpha') = ((1, 2, 3, 4, 5), (1, 3, 5, 2, 4))$ with $(\beta, \beta') = (\alpha, \alpha')$ along $s = (1, 2, 3)$, $t = (4, 2, 5)$. Here, $X = \{1, 2, 3, 4, 5\}$, $Y = \{1, 2, 3, 4, 5\}$ and $Z = \{1, 2, \dots, 7\}$. The elements $1, 2, 3, 4, 5$ of Y are identified with the elements $1, 2, 3, 4, 5$ of Z, and the elements $1, 2, 3, 4, 5$ of X are identified with the elements $4, 2, 5, 6, 7$ of Z. In other words, we replace (α, α') with $(\alpha, \alpha') = ((4, 2, 5, 6, 7), (4, 5, 7, 2, 6))$. In order to obtain γ, we shuffle $\alpha = (4, 2, 5, 6, 7)$ and $\beta = (1, 2, 3, 4, 5)$ such that both dihedral structures are preserved (because of the conditions of multipliability there is a unique such shuffle). The result is $\gamma = (1, 2, 3, 4, 7, 6, 5)$. Likewise, shuffling $\alpha' = (4, 5, 7, 2, 6)$ and $\beta' = (1, 3, 5, 2, 4)$ results in $\gamma' = (1, 3, 5, 7, 2, 6, 4)$. We refer to [**13**, example 6·3] for another example accompanied by a helpful illustration.

The main interest in this partial multiplication stems from the following result. For its statement, recall that every configuration $[\gamma, \gamma']$ can be represented as $[\sigma] = [\mathrm{id}, \sigma]$. Since, up to a sign, the cellular integral I_σ only depends on the configuration $[\sigma]$, we may write $I_{[\gamma,\gamma']} = I_\sigma$. Likewise, we write $A_{[\gamma,\gamma']} = A_\sigma$ for the corresponding leading coefficients.

PROPOSITION 2·2 [**13**, proposition 6·5]. *Suppose that*

$$(\gamma, \gamma') = (\alpha, \alpha') \star_{s,t} (\beta, \beta')$$

for some choice of s, t. *Then, for all* $n \geqslant 0$, *possibly up to a sign,*

$$I_{[\gamma,\gamma']}(n) = I_{[\alpha,\alpha']}(n) I_{[\beta,\beta']}(n).$$

In particular, $A_{[\gamma,\gamma']}(n) = A_{[\alpha,\alpha']}(n) A_{[\beta,\beta']}(n)$.

Example 2·3. Recall that, for $\sigma_5 = (1, 3, 5, 2, 4)$, the leading terms $A_{\sigma_5}(n)$ of the corresponding cellular integrals are the Apéry numbers $a(n)$. The configuration $[\sigma_5]$ is represented

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by the pairs of dihedral structures $(\alpha, \alpha') = (\beta, \beta')$ from Example 2·1. Let (γ, γ') be the product of these two pairs along s, t as chosen in Example 2·1. Observe that, as a configuration, $[\gamma, \gamma'] = [\sigma_7]$ with $\sigma_7 = (1, 3, 7, 5, 2, 6, 4)$. By Proposition 2·2, $A_{\sigma_7}(n) = a(n)^2$.

Similarly, many leading coefficients $A_\sigma(n)$ are products of leading coefficients of lower order. However, it is not the case that products of leading coefficients are always leading coefficients.

Example 2·4. Consider the configuration $\sigma_8 = (8, 3, 6, 1, 4, 7, 2, 5)$ featured in Theorem 1·2 and Section 3. This configuration is self-dual and not multipliable along any choice of triple t. Indeed, we confirm numerically that the product $a(n)A_{\sigma_8}(n)$ is not a leading coefficient $A_{\sigma_{10}}(n)$ for any configuration σ_{10}.

Nevertheless, the next result guarantees that all positive integer powers of the Apéry numbers $a(n)$ are leading coefficients.

PROPOSITION 2·5. *If* $\rho = (N-1, \rho_0, N, \rho_1, \rho_2, \ldots, \rho_{N-3}) \in \Sigma_N$, *then*

$$A_\tau(n) = a(n)A_\rho(n),$$

where $\tau = (N+1, \rho_0+1, N+2, N, \rho_{N-3}+1, \rho_{N-4}+1, \ldots, \rho_1+1, 1)$.

Note that τ is of the same shape of ρ, so that the result can be iterated to conclude that $a(n)^\lambda A_\rho(n)$ is a leading coefficient for any integer $\lambda \geqslant 0$.

Proof. Let $(\alpha, \alpha') = ((1, 2, 3, 4, 5), (1, 3, 5, 2, 4))$ and $(\beta, \beta') = ((1, 2, \ldots, N), \rho)$. Note that (α, α') is multipliable along $s = (1, 2, 3)$, and that the dual of (β, β') is multipliable along $t = (N-1, \rho_0, N)$. Let $(\gamma, \gamma') = (\alpha, \alpha') \star_{s,t} (\beta, \beta')$.

To compute this product, we proceed as in Example 2·1 and replace (α, α') with $(\alpha, \alpha') = ((N-1, \rho_0, N, N+1, N+2), (N-1, N, N+2, \rho_0, N+1))$. Then, shuffling $\alpha = (N-1, \rho_0, N, N+1, N+2)$ and $\beta = (1, 2, \ldots, N)$ such that both dihedral structures are preserved, we obtain

$$\gamma = (1, 2, \ldots, N-1, N+2, N+1, N).$$

Likewise, shuffling $\alpha' = (N-1, N, N+2, \rho_0, N+1)$ and $\beta' = (N-1, \rho_0, N, \rho_1, \rho_2, \ldots, \rho_{N-3})$ results in

$$\gamma' = (N-1, N+1, \rho_0, N+2, N, \rho_1, \rho_2, \ldots, \rho_{N-3}).$$

Since $[\alpha, \alpha'] = [\sigma_5]$ and $[\beta, \beta'] = [\rho]$, Proposition 2·2 implies that

$$A_{[\gamma,\gamma']}(n) = a(n)A_\rho(n),$$

so that it only remains to observe that $[\gamma, \gamma'] = [\tau]$. First, swapping N and $N+2$, we find that

$$[\gamma, \gamma'] = [(N-1, N+1, \rho_0, N, N+2, \rho_1, \rho_2, \ldots, \rho_{N-3})].$$

Finally, as configurations, we have

$$\begin{aligned}
&[(N-1, N+1, \rho_0, N, N+2, \rho_1, \rho_2, \ldots, \rho_{N-3})] \\
&\quad = [(N, N+2, \rho_0+1, N+1, 1, \rho_1+1, \rho_2+1, \ldots, \rho_{N-3}+1)] \\
&\quad = [(N+1, \rho_0+1, N+2, N, \rho_{N-3}+1, \rho_{N-4}+1, \ldots, \rho_1+1, 1)],
\end{aligned}$$

which is $[\tau]$, as claimed.

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Example 2·6. Let us illustrate with $\rho = (4, 2, 5, 3, 1)$. Since $A_\rho(n) = a(n)$, Proposition 2·5 implies that

$$A_{\sigma_7}(n) = a(n)^2, \quad \sigma_7 = (6, 3, 7, 5, 2, 4, 1).$$

Note that this configuration agrees with the one obtained in Example 2·3. Iterating Proposition 2·5, we find

$$A_{\sigma_9}(n) = a(n)^3, \quad \sigma_9 = (8, 4, 9, 7, 2, 5, 3, 6, 1),$$
$$A_{\sigma_{11}}(n) = a(n)^4, \quad \sigma_{11} = (10, 5, 11, 9, 2, 7, 4, 6, 3, 8, 1).$$

In fact, the family of configurations in Example 2·6 can be made explicit as follows. For a positive integer M and configuration $(a_1, a_2, \ldots, a_N)$, we write $M + (a_1, a_2, \ldots, a_N)$ for $(M + a_1, M + a_2, \ldots, M + a_N)$.

COROLLARY 2·7. *Let $M \geqslant 2$ be an integer. Then*

$$A_{\sigma_{2M+1}}(n) = a(n)^{M-1},$$

where the configuration σ_{2M+1} is

$$\sigma_{2M+1} = M + (M, 0, M+1, M-1, -(M-2), M-3, \ldots, \pm 1, \mp 1, \pm 2, \ldots, -(M-1)).$$

Proof. The statement is clearly true for $M = 2$, in which case $\sigma_5 = (4, 2, 5, 3, 1)$. The claim then follows from Proposition 2·5 by induction.

2·2. *Modular forms with complex multiplication and Hecke characters*

In this section, we recall some properties of modular forms with complex multiplication and Hecke characters. For more details, see [**39**].

Suppose ψ is a nontrivial real Dirichlet character with corresponding quadratic field K. A newform $f(z) = \sum_{n=1}^{\infty} \gamma(n) q^n$, where $q := e^{2\pi i z}$, has complex multiplication (CM) by ψ, or by K, if $\gamma(p) = \psi(p)\gamma(p)$ for all primes p in a set of density one.

By the work of Hecke and Shimura we can construct CM newforms using Hecke characters. Let $K = \mathbb{Q}(\sqrt{-d})$ be an imaginary quadratic field with discriminant D, and let $\mathcal{O}_K$ be its ring of integers. For an ideal $\mathfrak{f} \in \mathcal{O}_K$, let $I(\mathfrak{f})$ denote the group of fractional ideals prime to $\mathfrak{f}$. A Hecke character of weight k and modulo $\mathfrak{f}$ is a homomorphism $\Phi : I(\mathfrak{f}) \to \mathbb{C}^*$, satisfying $\Phi(\alpha\,\mathcal{O}_K) = \alpha^{k-1}$ when $\alpha \equiv^\times 1 \pmod{\mathfrak{f}}$. Let $N(\mathfrak{a})$ denote the norm of the ideal $\mathfrak{a}$. Then,

$$f(z) := \sum_{\mathfrak{a}} \Phi(\mathfrak{a}) q^{N(\mathfrak{a})} = \sum_{n=1}^{\infty} \gamma(n) q^n,$$

where the sum is over all ideals $\mathfrak{a}$ in $\mathcal{O}_K$ prime to $\mathfrak{f}$, is a Hecke eigenform of weight k on $\Gamma_0(|D| \cdot N(\mathfrak{f}))$ with Nebentypus $\chi(n) = \left(\frac{D}{n}\right) \frac{\Phi(n\,\mathcal{O}_K)}{n^{k-1}}$. Here, (a/n) is the Kronecker symbol. Furthermore, f has CM by K. We call $\mathfrak{f}$ the conductor of Φ if $\mathfrak{f}$ is minimal, i.e., if Φ is defined modulo $\mathfrak{f}'$ then $\mathfrak{f} \mid \mathfrak{f}'$. If $\mathfrak{f}$ is the conductor of Φ then $f(z)$ is a newform. From [**39**], we also know that every CM newform comes from a Hecke character in this way.

We will see that Theorem 1·1 is a consequence of Corollary 2·7 and Corollary 2·11.

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THEOREM 2·8. *Let $k \geqslant 2$ be a positive integer. Then there exists a weight k CM newform*

$$f_k(z) =: \sum_{n=1}^{\infty} \gamma_k(n) q^n \in \begin{cases} S_k(\Gamma_0(32)), & \text{if } k \text{ is even}, \\ S_k(\Gamma_0(4), (\frac{-4}{\cdot})), & \text{if } k \equiv 1 \pmod 4, \\ S_k(\Gamma_0(16), (\frac{-4}{\cdot})), & \text{if } k \equiv 3 \pmod 4, \end{cases}$$

such that, for any odd prime p,

$$\gamma_k(p) = \begin{cases} (-1)^{\frac{(x+y-1)(k-1)}{2}} \left[(x+iy)^{k-1} + (x-iy)^{k-1}\right], & \text{if } p = x^2 + y^2, \ x \text{ odd}, \\ 0, & \text{if } p \equiv 3 \pmod 4. \end{cases}$$

Proof. For k in each equivalence class modulo 4, we will define a Hecke character Ψ_k and construct the required CM newform f_k, using the methodology outlined above.

For an ideal $\mathfrak{f} \in \mathcal{O}_K$, let $I(\mathfrak{f})$ denote the group of fractional ideals prime to $\mathfrak{f}$, and let $J(\mathfrak{f})$ be the subset of principal fractional ideals whose generator is multiplicatively congruent to 1 modulo $\mathfrak{f}$, i.e., $J(\mathfrak{f}) = \{(\alpha) \in I(\mathfrak{f}) \mid \alpha \equiv^{\times} 1 \pmod{\mathfrak{f}}\}$.

Let $K = \mathbb{Q}(\sqrt{-1})$ which has discriminant $D = -4$ and whose ring of integers is $\mathcal{O}_K = \mathbb{Z}[\sqrt{-1}]$, which is a principal ideal domain. Therefore, all fractional ideals of K are also principal, and are of the form $\frac{1}{m}(\alpha)$ where $m \in \mathbb{Z} \setminus \{0\}$ and $\alpha \in \mathcal{O}_K$.

Case 1. $k \equiv 1 \pmod 4$. Let $\mathfrak{f} = (1)$. Then $I(\mathfrak{f}) = J(\mathfrak{f})$ is the set of all fractional ideals. We define the Hecke character $\Phi_k : I((1)) \to \mathbb{C}^*$ of weight k and conductor (1) by

$$\Phi_k\left(\frac{1}{m}(\alpha)\right) = \left(\frac{\alpha}{m}\right)^{k-1}.$$

Therefore,

$$f_k(z) := \sum_{\mathfrak{a}} \Phi_k(\mathfrak{a}) q^{N(\mathfrak{a})} = \sum_{n=1}^{\infty} \gamma_k(n) q^n \in S_k(\Gamma_0(4), (\tfrac{-4}{\cdot}))$$

is a CM newform and, for p an odd prime,

$$\gamma_k(p) = \begin{cases} (x+iy)^{k-1} + (x-iy)^{k-1}, & \text{if } p \equiv 1 \pmod 4, \ p = x^2 + y^2, \ x \text{ odd}, \\ 0, & \text{if } p \equiv 3 \pmod 4. \end{cases}$$

Case 2. $k \equiv 3 \pmod 4$. Let $\mathfrak{f} = (2)$. Then

$$I((2)) = \left\{ \frac{1}{m}(\alpha) \mid m \in \mathbb{Z} \text{ odd}, \alpha = x + iy \in \mathbb{Z}[\sqrt{-1}], x \text{ and } y \text{ different parity} \right\}$$

and

$$J((2)) = \left\{ \frac{1}{m}(\alpha) \mid m \in \mathbb{Z} \text{ odd}, \alpha = x + iy \in \mathbb{Z}[\sqrt{-1}], x \text{ odd}, y \text{ even} \right\}.$$

We define the Hecke character $\Phi_k : I((2)) \to \mathbb{C}^*$ of weight k and conductor (2) by

$$\Phi_k\left(\frac{1}{m}(x+iy)\right) = \left(\frac{x+iy}{m}\right)^{k-1} \cdot (-1)^y.$$

Therefore,

$$f_k(z) := \sum_{\mathfrak{a}} \Phi_k(\mathfrak{a}) q^{N(\mathfrak{a})} = \sum_{n=1}^{\infty} \gamma_k(n) q^n \in S_k\left(\Gamma_0(16), \left(\frac{-4}{\cdot}\right)\right)$$

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is a CM newform, and for p an odd prime,

$$\gamma_k(p) = \begin{cases} (x+iy)^{k-1} + (x-iy)^{k-1}, & \text{if } p \equiv 1 \pmod 4,\ p = x^2+y^2,\ x \text{ odd}, \\ 0, & \text{if } p \equiv 3 \pmod 4. \end{cases}$$

Case 3. k even. Let $\mathfrak{f} = (2+2i)$. Then

$$I((2+2i)) = \left\{ \frac{1}{m}(\alpha) \mid m \in \mathbb{Z} \text{ odd}, \alpha = x+iy \in \mathbb{Z}[\sqrt{-1}], x \text{ and } y \text{ different parity} \right\}$$

and

$$J((2+2i)) = \left\{ \frac{1}{m}(\alpha) \mid m \in \mathbb{Z} \text{ odd}, \alpha = x+iy \in \mathbb{Z}[\sqrt{-1}], x \text{ odd}, y \text{ even, such that} \right.$$
$$\left. \text{if } m \equiv x \pmod 4 \text{ then } y \equiv 0 \pmod 4, \text{otherwise } y \equiv 2 \pmod 4 \right\}.$$

We define the Hecke character $\Phi_k : I((2+2i)) \to \mathbb{C}^*$ of weight k and conductor $(2+2i)$ by

$$\Phi_k\left(\frac{1}{m}(x+iy)\right) = \left(\frac{x+iy}{m}\right)^{k-1} \chi(x+iy)^{k-1} \cdot (-1)^y \cdot (-1)^{\frac{m-1}{2}},$$

where

$$\chi(x+iy) = (-1)^{\frac{x+y-1}{2}} \cdot \begin{cases} 1, & \text{if } x \text{ odd}, y \text{ even}, \\ i, & \text{if } x \text{ even}, y \text{ odd}. \end{cases}$$

Therefore,

$$f_k(z) := \sum_{\mathfrak{a}} \Phi_k(\mathfrak{a}) q^{N(\mathfrak{a})} = \sum_{n=1}^{\infty} \gamma_k(n) q^n \in S_k(\Gamma_0(32))$$

is a CM newform and, for p an odd prime,

$$\gamma_k(p) = \begin{cases} (-1)^{\frac{x+y-1}{2}} \left[(x+iy)^{k-1} + (x-iy)^{k-1} \right], & \text{if } p = x^2+y^2 \equiv 1 \pmod 4,\ x \text{ odd}, \\ 0, & \text{if } p \equiv 3 \pmod 4. \end{cases}$$

Remark 2·9. When k is odd, an alternative expression for the CM newform $f_k(z)$ constructed in Theorem 2·8 is given by the binary theta series

$$f_k(z) = \frac{1}{4} \sum_{(n,m) \in \mathbb{Z}^2} (-1)^{m(k-1)/2} (n-im)^{k-1} q^{n^2+m^2}. \tag{2·1}$$

The formulation (2·1) was recently used to relate the L-series of f_k at $k-1$ to an interpolated version of the leading coefficients in Corollary 2·7. For further details, see [**36**].

COROLLARY 2·10. *Let $k \geqslant 2$ be a positive integer and let $f_k(z) =: \sum_{n=1}^{\infty} \gamma_k(n) q^n$ be the weight k CM newform described in Theorem* 2·8. *Then, for any odd prime p and integer $m \geqslant 1$,*

$$\gamma_k(p)^m = \sum_{t=0}^{\lfloor \frac{m-1}{2} \rfloor} \binom{m}{t} p^{t(k-1)} \gamma_{(m-2t)(k-1)+1}(p)$$
$$+ \begin{cases} \binom{m}{\frac{m}{2}} p^{\frac{m}{2}(k-1)}, & \textit{if } p \equiv 1 \pmod 4 \textit{ and } m \textit{ even}, \\ 0, & \textit{otherwise}. \end{cases}$$

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Proof. This follows from a simple application of the binomial theorem on the expression for $\gamma_k(p)$ given in Theorem 2·8, while noting that $(-1)^{\frac{x+y-1}{2}}(x+iy)\cdot(-1)^{\frac{x+y-1}{2}}(x-iy) = p$.

COROLLARY 2·11. *Let $l \geqslant 1$ be a positive integer and define $k := 2l+1$. Let $f_k(z) =: \sum_{n=1}^{\infty}\gamma_k(n)q^n$ be the weight k CM newform described in Theorem 2·8. Let $a(n) = \sum_{j=0}^{n}\binom{n}{j}^2\binom{n+j}{j}$ be the Apéry numbers introduced in* (1·3). *Then, for primes $p \geqslant 5$,*

$$a\left(\frac{p-1}{2}\right)^l \equiv \gamma_k(p) \pmod{p^2}.$$

Proof. By (1·4) and Corollary 2·10,

$$a\left(\frac{p-1}{2}\right)^l \equiv \gamma_3(p)^l \equiv \gamma_k(p) \pmod{p^2}.$$

We can now prove Theorem 1·1.

Proof of Theorem 1·1. Let $l \geqslant 1$ be a positive integer and define $k = 2l+1$ and $N = 2l+3$. Consider $f_k(z) =: \sum_{n=1}^{\infty}\gamma_k(n)q^n$ as in Theorem 2·8. By Corollary 2·7, there exists a convergent σ_N whose leading coefficient $A_{\sigma_N}(n)$ satisfies

$$A_{\sigma_N}(n) = a(n)^l. \tag{2·2}$$

Thus, the result then follows from (2·2) and Corollary 2·11.

3. *Multiple binomial sums*

3·1. *Proving multiple binomial sum representations for $A_\sigma(n)$*

In this section, we outline how to obtain multiple binomial sum representations for the leading coefficients $A_\sigma(n)$. Our discussion applies to any configuration, but we proceed with the configuration $\sigma_8 = (8,3,6,1,4,7,2,5)$ for $N = 8$ which is relevant to Theorem 1·2. This is the self-dual configuration ${}_8\pi_6$ in Brown's notation [**13**, section 10·1·4]. The leading coefficients $A_{\sigma_8}(n)$ have initial terms

$$1, 33, 8929, 4124193, 2435948001, 1657775448033, \ldots$$

and the following particularly symmetric binomial sum representation.

PROPOSITION 3·1. *For the configuration $\sigma_8 = (8,3,6,1,4,7,2,5)$, the leading coefficients are*

$$A_{\sigma_8}(n) = \sum_{\substack{k_1,k_2,k_3,k_4=0\\ k_1+k_2=k_3+k_4}}^{n}\prod_{i=1}^{4}\binom{n}{k_i}\binom{n+k_i}{k_i}. \tag{3·1}$$

Proof. For $\sigma = \sigma_8$, consider the cellular integral $I_\sigma(n) = \int_{S_8} f_\sigma^n\,\omega_\sigma$ where

$$f_\sigma = \frac{(z_1-z_2)(z_2-z_3)(z_3-z_4)(z_4-z_5)(z_5-z_6)(z_6-z_7)(z_7-z_8)(z_8-z_1)}{(z_8-z_3)(z_3-z_6)(z_6-z_1)(z_1-z_4)(z_4-z_7)(z_7-z_2)(z_2-z_5)(z_5-z_8)}. \tag{3·2}$$

As in Section 1, we let $z_1 = 0$, $z_7 = 1$, $z_8 = \infty$. Then, in the coordinates $t_1 = z_2, t_2 = z_3, t_3 = z_4, t_4 = z_5, t_5 = z_6$, we have

$$f_\sigma = \frac{(-t_1)(t_1-t_2)(t_2-t_3)(t_3-t_4)(t_4-t_5)(t_5-1)}{(t_2-t_5)(t_5)(-t_3)(t_3-1)(1-t_1)(t_1-t_4)},$$

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and

$$\omega_\sigma = \frac{dt_1dt_2dt_3dt_4dt_5}{(t_2-t_5)(t_5)(-t_3)(t_3-1)(1-t_1)(t_1-t_4)}.$$

The domain S_8 of integration then consists of all $(t_1, t_2, \dots, t_5) \in \mathbb{R}^5$ such that $0 < t_1 < t_2 < \cdots < t_5 < 1$. Algorithmic approaches to computing explicit period integrals, such as $I_\sigma(n)$ for specific values of n, are described in [**10**] or [**37**]. In particular, Panzer implemented his symbolic integration approach [**37**] using hyperlogarithms in a Maple package called `HyperInt`. Using this package, we explicitly evaluate $I_\sigma(n)$ in terms of multiple zeta values for several small values of n, and obtain:

$$\begin{aligned}
I_\sigma(0) &= 16\zeta(5) - 8\zeta(3)\zeta(2)\\
I_\sigma(1) &= 33I_\sigma(0) - 432\zeta(3) + 316\zeta(2) - 26\\
I_\sigma(2) &= 8929I_\sigma(0) - 117500\zeta(3) + \tfrac{515189}{6}\zeta(2) - \tfrac{331063}{48}\\
I_\sigma(3) &= 4124193I_\sigma(0) - 54272204\zeta(3) + \tfrac{10708231609}{270}\zeta(2) - \tfrac{12385477271}{3888}\\
I_\sigma(4) &= 2435948001I_\sigma(0) - 32055790815\zeta(3) + \tfrac{23612586361625}{1008}\zeta(2) - \tfrac{78031593554765}{41472}.
\end{aligned}$$

As proven by Brown in [**13**, section 4], the integrals $I_\sigma(n)$ satisfy a linear recurrence with polynomial coefficients. Slightly more specifically, the ordinary generating function

$$F_\sigma(x) := \sum_{n=0}^{\infty} I_\sigma(n)x^n$$

satisfies a Picard–Fuchs differential equation. Again, in each specific instance, this differential equation can be obtained algorithmically. A particularly efficient such approach is an extension of the Griffiths–Dwork reduction method due to Lairez [**28**] for computing periods of rational functions. To apply this method, we observe that

$$F_\sigma(x) = \int_{S_8} \frac{\omega_\sigma}{1-f_\sigma x} = \int_{S_8} \frac{dt_1dt_2dt_3dt_4dt_5}{A-Bx},$$

where

$$\begin{aligned}
A &= (t_2-t_5)(t_5)(-t_3)(t_3-1)(1-t_1)(t_1-t_4),\\
B &= (-t_1)(t_1-t_2)(t_2-t_3)(t_3-t_4)(t_4-t_5)(t_5-1).
\end{aligned}$$

Lairez's method (implemented in Magma) then successfully determines a Fuchsian differential equation of order 7 satisfied by $F_\sigma(x)$. This differential equation has a two-dimensional space of analytic solutions around $x = 0$. As a consequence, this differential equation together with the two values $I_\sigma(0)$, $I_\sigma(1)$, explicitly obtained above, determines the values of the cellular integrals $I_\sigma(n)$ for all $n \geqslant 2$.

Alternatively, the differential equation for the generating function $F_\sigma(x)$ translates directly into a recurrence of order 12 for the coefficients $I_\sigma(n)$ and, hence, for the leading coefficients $A_\sigma(n)$. That is, we find that

$$1521n(n+1)^5(2n+1)A_\sigma(n+1) = \sum_{j=0}^{11} q_j(n)A_\sigma(n-j)$$

for certain polynomials $q_j(x) \in \mathbb{Z}[x]$ of degree 7. To complete the proof, it therefore only

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remains to verify that the numbers

$$B_\sigma(n) := \sum_{\substack{k_1,k_2,k_3,k_4=0 \\ k_1+k_2=k_3+k_4}}^{n} \prod_{i=1}^{4} \binom{n}{k_i}\binom{n+k_i}{n}$$

satisfy the same recurrence with matching initial values. This can be done algorithmically using, for instance, creative telescoping. In practice, the fact that $B_\sigma(n)$ is a triple sum makes the computation of the recurrence rather challenging. Yet, Koutschan's Mathematica package `HolonomicFunctions` [**27**] is able to determine a fourth order linear recurrence for $B_\sigma(n)$ (see below for more information on this recurrence). We then verify that this recurrence is a right factor of the earlier recurrence of order 12 for $A_\sigma(n)$. Since the first 12 initial values match (in fact, additional reflection shows that two matching initial values suffice), we conclude that $A_\sigma(n) = B_\sigma(n)$.

The proof of Proposition 3·1 demonstrates that any individual evaluation of leading coefficients in terms of binomial sums can, in principle, be algorithmically proven due to recent advances in symbolic computation. It is curious to note that we had to use Maple, Magma and Mathematica in that computation.

Remark 3·2. We find that $A_{\sigma_8}(n)$, with σ_8 as in Proposition 3·1, is the unique solution of a fourth order recurrence

$$p_4(n)a_{n+4} + p_3(n)a_{n+3} + p_2(n)a_{n+2} + p_1(n)a_{n+1} + p_0(n)a_n = 0,$$

with initial conditions $a_0 = 1, a_1 = 33$ and $a_j = 0$ for $j < 0$. Here, the coefficients $p_j(n)$ are polynomials of degree 15, satisfying

$$p_j(n) = -p_{4-j}(-5-n),$$

for $j \in \{1, 2, 3, 4\}$. The latter relation is a consequence of the fact that the configuration σ_8 is self-dual (see [**13**, section 4]).

3·2. *Finding multiple binomial sum representations for* $A_\sigma(n)$

In this section, we illustrate how binomial sum representations can be found for any convergent configuration σ. As in the previous section, we proceed with the configuration $\sigma = \sigma_8 = (8, 3, 6, 1, 4, 7, 2, 5)$. Consider the cellular integral

$$I_\sigma(n) = \int_{S_8} f_\sigma^n \, \omega_\sigma,$$

where f_σ is as in (3·2). Because the action of PGL_2 is triply transitive, we may also make the convenient choice $z_{\sigma(6)} = z_7 = 1$, $z_{\sigma(7)} = z_2 = 0$, $z_{\sigma(8)} = z_5 = \infty$. Then, in the coordinates $t_1 = z_1, t_2 = z_3, t_3 = z_4, t_4 = z_6, t_5 = z_8$, we have

$$f_\sigma = \frac{(t_1)(-t_2)(t_2-t_3)(t_4-1)(1-t_5)(t_5-t_1)}{(t_5-t_2)(t_2-t_4)(t_4-t_1)(t_1-t_3)(t_3-1)}$$

and

$$\omega_\sigma = \frac{dt_1dt_2dt_3dt_4dt_5}{(t_5-t_2)(t_2-t_4)(t_4-t_1)(t_1-t_3)(t_3-1)}.$$

We then substitute

$$x_1 = t_5 - t_2, \quad x_2 = t_2 - t_4, \quad x_3 = t_4 - t_1, \quad x_4 = t_1 - t_3, \quad x_5 = t_3 - 1.$$

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Observe that $t_3 = x_5 + 1$, $t_1 = x_4 + x_5 + 1$ and, likewise,

$$t_4 = x_3 + x_4 + x_5 + 1, \quad t_2 = x_2 + x_3 + x_4 + x_5 + 1, \quad t_5 = x_1 + x_2 + x_3 + x_4 + x_5 + 1,$$

so that, up to a sign in ω_σ,

$$f_\sigma = \frac{x_{4,6}x_{2,6}x_{2,4}x_{3,5}x_{1,5}x_{1,3}}{x_1x_2x_3x_4x_5},$$
$$\omega_\sigma = \frac{dx_1dx_2dx_3dx_4dx_5}{x_1x_2x_3x_4x_5},$$

where $x_{i,j} = x_i + x_{i+1} + \ldots + x_j$ with $x_6 = 1$.

At this point, it is natural to also consider the integral

$$J_\sigma(n) = \frac{1}{(2\pi i)^5} \oint_{|x_i|=\varepsilon} f_\sigma^n \omega_\sigma$$
$$= \frac{1}{(2\pi i)^5} \oint_{|x_i|=\varepsilon} \left(\frac{x_{4,6}x_{2,6}x_{2,4}x_{3,5}x_{1,5}x_{1,3}}{x_1x_2x_3x_4x_5}\right)^n \frac{dx_1dx_2dx_3dx_4dx_5}{x_1x_2x_3x_4x_5},$$

where ε is chosen sufficiently small so that the integrals converge. By the residue theorem, this integral evaluates to

$$J_\sigma(n) = [(x_1x_2x_3x_4x_5)^n](x_{4,6}x_{2,6}x_{2,4}x_{3,5}x_{1,5}x_{1,3})^n.$$

In particular, the values $J_\sigma(n)$ are nonnegative integers. By the principle of creative telescoping, we can derive a linear recurrence which is satisfied by both $I_\sigma(n)$ and $J_\sigma(n)$. In fact, we are going to show that the leading coefficients $A_\sigma(n)$ of $I_\sigma(n)$ are equal to $J_\sigma(n)$. Likely, one can prove this equality in a general uniform fashion (for instance, following the approach of [**18**], as suggested by Dupont). For our purposes, it suffices to observe that both sequences satisfy a common recurrence and agree to sufficiently many terms. It remains to express $J_\sigma(n)$ in terms of a multiple binomial sum.

Here, it will be convenient to not specialise x_6. In order to find an explicit formula for $J_\sigma(n)$, we expand

$$\Lambda = (x_{1,5}x_{2,6}x_{1,3}x_{2,4}x_{3,5}x_{4,6})^n$$

using the binomial theorem and then extract the coefficient of $(x_1x_2x_3x_4x_5x_6)^n$. Some care needs to be applied at this stage, because the order in which terms are expanded can have a considerable influence on the final binomial sum. For instance, the number of summations can vary substantially. In the present case, it is natural to first expand

$$x_{1,5}^n = \sum_{k_1=0}^n \binom{n}{k_1} x_{1,3}^{k_1} x_{4,5}^{n-k_1}, \quad x_{2,6} = \sum_{k_2=0}^n \binom{n}{k_2} x_{4,6}^{k_2} x_{2,3}^{n-k_2},$$

and, in a second step, $x_{1,3}^{n+k_1}$ as well as $x_{4,6}^{n+k_4}$, so that Λ equals

$$\sum_{k_1,k_4} \binom{n}{k_1}\binom{n}{k_4} x_{1,3}^{n+k_1} x_{2,4}^n x_{3,5}^n x_{4,6}^{n+k_4} x_{2,3}^{n-k_4} x_{4,5}^{n-k_1}$$
$$= \sum_{k_1,k_4,\ell_1,\ell_4} \binom{n}{k_1}\binom{n}{k_4}\binom{n+k_1}{\ell_1}\binom{n+k_4}{\ell_4} x_{2,4}^n x_{3,5}^n x_{2,3}^{n-k_4+\ell_1} x_{4,5}^{n-k_1+\ell_4} x_1^{n+k_1-\ell_1} x_6^{n+k_4-\ell_4}.$$

Since $J_\sigma(n)$ is the coefficient of $(x_1x_2x_3x_4x_5x_6)^n$ in Λ, we conclude that $J_\sigma(n)$ is the coeffi-

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cient of $(x_2x_3x_4x_5)^n$ in

$$\sum_{k_1,k_4}\binom{n}{k_1}\binom{n}{k_4}\binom{n+k_1}{k_1}\binom{n+k_4}{k_4}x_{2,4}^n x_{3,5}^n x_{2,3}^{n-k_4+k_1}x_{4,5}^{n-k_1+k_4}. \tag{3·3}$$

We next expand $x_{2,4}^n$ and $x_{3,5}^n$ to obtain

$$\begin{aligned}
&x_{2,4}^n x_{3,5}^n x_{2,3}^{n-k_4+k_1}x_{4,5}^{n-k_1+k_4}\\
&\quad=\sum_{k_2,k_3}\binom{n}{k_2}\binom{n}{k_3}x_{2,3}^{n-k_4+k_1+k_2}x_{4,5}^{n-k_1+k_4+k_3}x_3^{n-k_3}x_4^{n-k_2}\\
&\quad=\sum_{k_2,k_3,\ell_2,\ell_3}\binom{n}{k_2}\binom{n}{k_3}\binom{n-k_4+k_1+k_2}{\ell_2}\binom{n-k_1+k_4+k_3}{\ell_3}\\
&\qquad\times x_2^{\ell_2}x_3^{n-k_3+n-k_4+k_1+k_2-\ell_2}x_4^{n-k_2+n-k_1+k_4+k_3-\ell_3}x_5^{\ell_3}.
\end{aligned}$$

The coefficient of $(x_2x_3x_4x_5)^n$ in that sum is

$$\sum_{k_2,k_3}\binom{n}{k_2}\binom{n}{k_3}\binom{n+k_2}{n}\binom{n+k_3}{n},$$

subject to the constraint $k_1+k_2=k_3+k_4$. Finally, combined with (3·3), we conclude that

$$J_\sigma(n)=\sum_{\substack{k_1,k_2,k_3,k_4=0\\ k_1+k_2=k_3+k_4}}^{n}\prod_{i=1}^{4}\binom{n}{k_i}\binom{n+k_i}{n},$$

which is the binomial sum of Proposition 3·1. A similar procedure has been carried out to find explicit binomial expressions for the remaining 897 leading coefficients $A_{\sigma_N}(n)$ for $7\leqslant N\leqslant 10$. Again, these expressions are available upon request.

4. *Proof of Theorem* 1·2

4·1. *Congruences for binomial coefficients and harmonic sums*

For a nonnegative integer n, we define the harmonic sum H_n by

$$H_n:=\sum_{j=1}^{n}\frac{1}{j}$$

and $H_0:=0$. We first recall some elementary congruences (see [**24**, section 7·7, theorems 133, 132, 116]): For p an odd prime, we have

$$\left(\frac{p-1}{2}\right)!^4\equiv 1 \pmod p, \tag{4·1}$$

$$\binom{p-1}{\frac{p-1}{2}}\equiv(-1)^{\frac{p-1}{2}}2^{2p-2} \pmod{p^2}, \tag{4·2}$$

$$2^{p-1}-1\equiv p\left(1+\frac{1}{3}+\frac{1}{5}\cdots+\frac{1}{p-2}\right) \pmod{p^2} \tag{4·3}$$

and, for primes $p>3$,

$$H_{p-1}\equiv 0 \pmod{p^2}. \tag{4·4}$$

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We will also need the following result, which follows easily from (4·3) and (4·4).

LEMMA 4·1. *For a prime $p > 3$,*

$$2^{2p-2} \equiv 1 - pH_{\frac{p-1}{2}} \pmod{p^2}.$$

For nonnegative integers n, let $(a)_n := a(a+1)(a+2)\cdots(a+n-1)$ denote the rising factorial, with $(a)_0 := 1$. Let p be an odd prime. We note that, for $0 \leqslant k \leqslant (p-1)/2$,

$$\binom{\frac{p-1}{2}+k}{k} \equiv \frac{(1+k)(2+k)\cdots(\frac{p-1}{2}+k)}{(\frac{p-1}{2})!} \equiv \frac{(k+1)_{\frac{p-1}{2}}}{(\frac{p-1}{2})!} \pmod{p},$$

and, similarly,

$$\binom{\frac{p-1}{2}}{k}\binom{\frac{p-1}{2}+k}{k} \equiv (-1)^k \left(\frac{(k+1)_{\frac{p-1}{2}}}{(\frac{p-1}{2})!}\right)^2 \pmod{p}, \tag{4·5}$$

as well as

$$\binom{p-1-k}{\frac{p-1}{2}} \equiv (-1)^{\frac{p-1}{2}} \binom{\frac{p-1}{2}+k}{k} \pmod{p}. \tag{4·6}$$

LEMMA 4·2. *For p an odd prime,*

$$\sum_{k=0}^{p-1} (k+1)^2_{\frac{p-1}{2}} \equiv -1 \pmod{p}.$$

Proof. Let $m := (p-1)/2$ and write

$$(k+1)^2_m = b_0 + \sum_{t=1}^{2m} b_t k^t$$

for appropriate integers b_t. Recall that, for positive integers s,

$$\sum_{j=1}^{p-1} j^s \equiv \begin{cases} -1 \pmod{p}, & \text{if } (p-1)|s\,, \\ \ \ 0 \pmod{p}, & \text{otherwise}\,. \end{cases} \tag{4·7}$$

Therefore,

$$\sum_{k=0}^{p-1} (k+1)^2_m = p\,b_0 + \sum_{k=0}^{p-1}\sum_{t=1}^{2m} b_t k^t = p\,b_0 + \sum_{t=1}^{2m} b_t \sum_{k=1}^{p-1} k^t \equiv -b_{p-1} \pmod{p}.$$

Since $(k+1)^2_m$ is monic, $b_{p-1} = 1$.

LEMMA 4·3. *For p an odd prime,*

$$\sum_{\substack{k_1,k_2,k_3,k_4=0 \\ \sum k_i = p-1}}^{\frac{p-1}{2}} \left[\prod_{i=1}^{4} (k_i+1)^2_{\frac{p-1}{2}}\right] \left(H_{\frac{p-1}{2}+k_4} - H_{k_4}\right) \equiv 0 \pmod{p}. \tag{4·8}$$

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Proof. For brevity, we again write $m = (p-1)/2$. Let $0 \leqslant k \leqslant (p-1)/2$ and consider

$$\begin{aligned}(m-k+1)_m &= \left(\frac{p-1}{2}-k+1\right)\left(\frac{p-1}{2}-k+2\right)\cdots(p-2-k)(p-1-k)\\ &\equiv \left(-\frac{p-1}{2}-k\right)\left(-\frac{p-1}{2}+1-k\right)\cdots(-2-k)(-1-k)\\ &\equiv (-1)^m(k+1)_m \pmod{p}.\end{aligned}$$

Similarly,

$$\begin{aligned}H_{2m-k}-H_{m-k} &= \frac{1}{p-1-k}+\frac{1}{p-2-k}+\cdots+\frac{1}{\frac{p-1}{2}-k+2}+\frac{1}{\frac{p-1}{2}-k+1}\\ &\equiv \frac{1}{-1-k}+\frac{1}{-2-k}+\cdots+\frac{1}{-\frac{p-1}{2}-k+1}+\frac{1}{-\frac{p-1}{2}-k}\\ &\equiv -(H_{m+k}-H_k) \pmod{p}.\end{aligned}$$

Let

$$S=\sum_{\substack{k_1,k_2,k_3,k_4=0\\ \sum k_i=p-1}}^{m}\left[\prod_{i=1}^{4}(k_i+1)_m^2\right]\left(H_{m+k_4}-H_{k_4}\right)$$

be the left-hand side of (4·8). By replacing k_i with $m-k_i$, for $i\in\{1,2,3,4\}$, we see that

$$S=\sum_{\substack{k_1,k_2,k_3,k_4=0\\ \sum k_i=p-1}}^{m}\left[\prod_{i=1}^{4}(m-k_i+1)_m^2\right]\left(H_{2m-k_4}-H_{m-k_4}\right)\equiv -S \pmod{p}.$$

Hence, the sum S must vanish modulo p.

LEMMA 4·4. *For p an odd prime,*

$$\sum_{\substack{k_1,k_2,k_3,k_4=0\\ \sum k_i=p-1}}^{\frac{p-1}{2}}\prod_{i=1}^{4}\binom{\frac{p-1}{2}}{k_i}\binom{\frac{p-1}{2}+k_i}{k_i}\equiv\sum_{\substack{k_1,k_2,k_3,k_4=0\\ k_1+k_2=k_3+k_4}}^{\frac{p-1}{2}}\prod_{i=1}^{4}\binom{\frac{p-1}{2}}{k_i}\binom{\frac{p-1}{2}+k_i}{k_i} \pmod{p^2}.$$

Proof. Once more, $m:=(p-1)/2$. Replacing k_1 and k_2 with $m-k_1$ and $m-k_2$, respectively, yields

$$\sum_{\substack{k_1,k_2,k_3,k_4=0\\ \sum k_i=p-1}}^{m}\prod_{i=1}^{4}\binom{m}{k_i}\binom{m+k_i}{k_i}=\sum_{\substack{k_1,k_2,k_3,k_4=0\\ k_1+k_2=k_3+k_4}}^{m}\prod_{i=1}^{2}\binom{m}{k_i}\binom{2m-k_i}{m-k_i}\prod_{i=3}^{4}\binom{m}{k_i}\binom{m+k_i}{k_i}.$$

Let $\underline{k}:=(k_1,k_2,k_3,k_4)$ and define

$$f(p,\underline{k}):=\prod_{i=1}^{2}\binom{m}{k_i}\binom{2m-k_i}{m-k_i}\prod_{i=3}^{4}\binom{m}{k_i}\binom{m+k_i}{k_i}$$

and

$$g(p,\underline{k}):=\prod_{i=1}^{4}\binom{m}{k_i}\binom{m+k_i}{k_i}.$$

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Then it suffices to prove

$$\sum_{\substack{k_1,k_2,k_3,k_4=0\\ k_1+k_2=k_3+k_4}}^{m} f(p,\underline{k}) \equiv \sum_{\substack{k_1,k_2,k_3,k_4=0\\ k_1+k_2=k_3+k_4}}^{m} g(p,\underline{k}) \pmod{p^2}.$$

It follows from (4·6) that

$$\binom{2m-k}{m-k} = \binom{2m-k}{m} \equiv (-1)^m \binom{m+k}{k} \pmod{p}.$$

Consequently, letting $m-\underline{k} := (m-k_1, m-k_2, m-k_3, m-k_4)$, we have that

$$\begin{aligned} &f(p,\underline{k}) + f(p, m-\underline{k}) - g(p,\underline{k}) - g(p, m-\underline{k}) \\ &\quad = \left[\prod_{i=1}^{4}\binom{m}{k_i}\right]\left[\prod_{i=1}^{2}\binom{2m-k_i}{m-k_i} - \prod_{i=1}^{2}\binom{m+k_i}{k_i}\right]\left[\prod_{i=3}^{4}\binom{m+k_i}{k_i} - \prod_{i=3}^{4}\binom{2m-k_i}{m-k_i}\right] \\ &\quad \equiv 0 \pmod{p^2}. \end{aligned}$$

Therefore,

$$\begin{aligned} &2\sum_{\substack{k_1,k_2,k_3,k_4=0\\ k_1+k_2=k_3+k_4}}^{m} \big[f(p,\underline{k}) - g(p,\underline{k})\big] \\ &\quad = \sum_{\substack{k_1,k_2,k_3,k_4=0\\ k_1+k_2=k_3+k_4}}^{m} \big[f(p,\underline{k}) + f(p, m-\underline{k}) - g(p,\underline{k}) - g(p, m-\underline{k})\big] \\ &\quad \equiv 0 \pmod{p^2}. \end{aligned}$$

4·2. *Multiplicative characters and finite field hypergeometric functions*

Let $\widehat{\mathbb{F}_p^*}$ denote the group of multiplicative characters of $\mathbb{F}_p^*$. We extend the domain of $\chi \in \widehat{\mathbb{F}_p^*}$ to $\mathbb{F}_p$, by defining $\chi(0) := 0$ (including the trivial character ε_p) and denote $\overline{\chi}$ as the inverse of χ. When p is odd we denote the character of order 2 of $\mathbb{F}_p^*$ by ϕ_p. We will drop the subscript p if it is clear from the context. We recall the following orthogonality relation. For $\chi \in \widehat{\mathbb{F}_p^*}$, we have

$$\sum_{x\in\mathbb{F}_p} \chi(x) = \begin{cases} p-1, & \text{if } \chi = \varepsilon, \\ 0, & \text{if } \chi \neq \varepsilon. \end{cases} \tag{4·9}$$

For $A, B \in \widehat{\mathbb{F}_p^*}$, let

$$\binom{A}{B} := \frac{B(-1)}{p} \sum_{x\in\mathbb{F}_p} A(x)\overline{B}(1-x).$$

Then, for $A_0, A_1, \ldots, A_n, B_1, \ldots, B_n \in \widehat{\mathbb{F}_p^*}$ and $x \in \mathbb{F}_p$, the finite field hypergeometric function of Greene [**23**] is defined as

$${}_{n+1}F_n\left(\begin{matrix} A_0, A_1, \ldots, A_n \\ B_1, \ldots, B_n \end{matrix}\middle| x\right)_p := \frac{p}{p-1} \sum_{\chi\in\widehat{\mathbb{F}_p^*}} \binom{A_0\chi}{\chi} \prod_{i=1}^{n} \binom{A_i\chi}{B_i\chi} \chi(x).$$

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We consider the case where $A_i = \phi_p$ for all i and $B_j = \varepsilon_p$ for all j and write

$$ {}_{n+1}F_n(x) = {}_{n+1}F_n\left(\begin{matrix}\phi_p, \phi_p, \ldots, \phi_p \\ \varepsilon_p, \ldots, \varepsilon_p\end{matrix}\,\middle|\, x\right)_p $$

for brevity.

Let $\mathbb{Z}_p$ denote the ring of p-adic integers and $\mathbb{Z}_p^*$ its group of units. We define the Teichmüller character to be the primitive character $\omega : \mathbb{F}_p \to \mathbb{Z}_p^*$ satisfying $\omega(x) \equiv x \pmod{p}$ for all $x \in \{0, 1, \ldots, p-1\}$. In fact,

$$ \omega(x) \equiv x^{p^{n-1}} \pmod{p^n} \tag{4·10} $$

for all $n \geqslant 1$.

Theorem 1·2 is now implied by Proposition 3·1 and the following result.

THEOREM 4·5. *Let*

$$ \eta^{12}(2z) =: \sum_{n=1}^{\infty} \gamma(n) q^n $$

be the unique newform in $S_6(\Gamma_0(4))$. *Then, for* p *an odd prime,*

$$ \gamma(p) \equiv \sum_{\substack{k_1,k_2,k_3,k_4=0 \\ k_1+k_2=k_3+k_4}}^{\frac{p-1}{2}} \prod_{i=1}^{4} \binom{\frac{p-1}{2}}{k_i}\binom{\frac{p-1}{2}+k_i}{k_i} \pmod{p^2}. \tag{4·11} $$

Proof. We confirm that (4·11) holds for $p = 3$ and assume $p \geqslant 5$ henceforth. For the Legendre family of elliptic curves E_λ, given by

$$ E_\lambda : y^2 = x(x-1)(x-\lambda), \qquad \lambda \notin \{0, 1\}, $$

we define

$$ a(p, \lambda) := p + 1 - \#E_\lambda(\mathbb{F}_p). $$

Then, from [**19**, proposition 2·1] and using the fact that $\dim(S_6(\Gamma_0(4))) = 1$, we get that for p an odd prime,

$$ \begin{aligned} \gamma(p) &= -3 - \sum_{\lambda=2}^{p-1} \left(a(p,\lambda)^4 - 3p\, a(p,\lambda)^2 + p^2\right) \\ &= -p^3 + 2p^2 - 3 - \sum_{\lambda=2}^{p-1} \left(a(p,\lambda)^4 - 3p\, a(p,\lambda)^2\right). \end{aligned} $$

From [**2**, lemma 2·1] we have

$$ \sum_{\lambda=2}^{p-1} a(p,\lambda)^2 = p^2 - 2p - 3, $$

so that, combining these two equations,

$$ \gamma(p) = 2p^3 - 4p^2 - 9p - 3 - \sum_{\lambda=2}^{p-1} a(p,\lambda)^4. \tag{4·12} $$

In [**26**, section 4], Koike showed that for $\lambda \neq 0, 1$,

$$ a(p,\lambda) = -\phi(-1) \cdot p \cdot {}_2F_1(\lambda). $$

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We now recall a couple of facts about finite field hypergeometric functions from [**30**, proposition 3] and [**23**, theorem 4·2] respectively:

$$p \cdot {}_2F_1(1) = -\phi(-1),$$

and, for $\lambda \neq 0$,

$${}_2F_1(\lambda) = \phi(\lambda) \cdot {}_2F_1\Big(\frac{1}{\lambda}\Big).$$

Therefore,

$$\begin{aligned}\sum_{\lambda=2}^{p-1} a(p,\lambda)^4 &= \sum_{\lambda=2}^{p-1} [-\phi(-1)\cdot p\cdot {}_2F_1(\lambda)]^4 \\ &= \sum_{\lambda=1}^{p-1} [-\phi(-1)\cdot p\cdot {}_2F_1(\lambda)]^4 - [-\phi(-1)\cdot p\cdot {}_2F_1(1)]^4 \\ &= \sum_{\lambda=1}^{p-1} [-\phi(-1)\cdot p\cdot {}_2F_1(\lambda)]^4 - 1 \\ &= \sum_{\lambda=1}^{p-1} \Big[-\phi(-\lambda)\cdot p\cdot {}_2F_1\Big(\frac{1}{\lambda}\Big)\Big]^4 - 1. \end{aligned} \tag{4·13}$$

By [**29**, theorem 2·4] (see also [**35**, theorem 1·1]) and (4·10), we get that, for $\lambda \neq 0$,

$$\begin{aligned}&-\phi(-\lambda)\cdot p\cdot {}_2F_1\Big(\frac{1}{\lambda}\Big) \\ &\quad = -\phi\left(-\frac{1}{\lambda}\right)\cdot p\cdot {}_2F_1\Big(\frac{1}{\lambda}\Big) \\ &\quad \equiv (p+1)\sum_{j=0}^{(p-1)/2} \binom{\frac{p-1}{2}}{j}\binom{\frac{p-1}{2}+j}{j}(-1)^j\lambda^{jp}\left(1+2jp\left(H_{\frac{p-1}{2}+j}-H_j\right)\right) \\ &\quad \equiv (p+1)\sum_{j=0}^{(p-1)/2} \binom{\frac{p-1}{2}}{j}\binom{\frac{p-1}{2}+j}{j} \\ &\qquad \times (-1)^j\left(1+2jp\left(H_{\frac{p-1}{2}+j}-H_j\right)\right)\omega(\lambda^j) \pmod{p^2}. \end{aligned} \tag{4·14}$$

For brevity, we again let $m = (p-1)/2$ and write

$$f(p,k_1,k_2,k_3,k_4) := \prod_{i=1}^{4}\binom{m}{k_i}\binom{m+k_i}{k_i}(-1)^{k_i}\left(1+2pk_i\left(H_{m+k_i}-H_{k_i}\right)\right).$$

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Combining (4·13) and (4·14) yields

$$1+\sum_{\lambda=2}^{p-1}a(p,\lambda)^4 \equiv \sum_{\lambda=1}^{p-1}\left[(p+1)\sum_{j=0}^{m}\binom{m}{j}\binom{m+j}{j}(-1)^j\left(1+2jp\left(H_{m+j}-H_j\right)\right)\omega^j(\lambda)\right]^4$$

$$\equiv (4p+1)\sum_{k_1,k_2,k_3,k_4=0}^{m} f(p,k_1,k_2,k_3,k_4)\sum_{\lambda=1}^{p-1}\omega^{k_1+k_2+k_3+k_4}(\lambda)$$

$$\equiv -(3p+1)\sum_{\substack{k_1,k_2,k_3,k_4=0\\ \sum k_i\equiv 0 \pmod{p-1}}}^{m} f(p,k_1,k_2,k_3,k_4) \pmod{p^2}, \tag{4·15}$$

where we have used (4·9) and the facts that $(p+1)^4 \equiv 4p+1 \pmod{p^2}$ and $(4p+1)(p-1) \equiv -(3p+1) \pmod{p^2}$. Accounting for (4·15) in (4·12), we now have

$$\gamma(p) \equiv -9p-2+(3p+1)\sum_{\substack{k_1,k_2,k_3,k_4=0\\ \sum k_i\equiv 0 \pmod{p-1}}}^{m} f(p,k_1,k_2,k_3,k_4) \pmod{p^2}.$$

In order that $\sum k_i \equiv 0 \pmod{p-1}$, the sum $\sum k_i$ must be either 0, $p-1$ or $2(p-1)$. In the case $\sum k_i = 0$, we necessarily have $k_1 = k_2 = k_3 = k_4 = 0$, which contributes $f(p,0,0,0,0) = 1$. In the third case, that is $\sum k_i = 2(p-1)$, we necessarily have $k_1 = k_2 = k_3 = k_4 = (p-1)/2 = m$. Applying (4·2), (4·4) and Lemma 4·1, we evaluate

$$f(p,m,m,m,m) = \left[\binom{m}{m}\binom{p-1}{m}(-1)^m\left(1+p(p-1)\left(H_{p-1}-H_m\right)\right)\right]^4$$

$$\equiv \left[\binom{p-1}{m}\left(1-p\left(H_{p-1}-H_m\right)\right)\right]^4$$

$$\equiv \left[(-1)^m 2^{2p-2}\left(1+pH_m\right)\right]^4$$

$$\equiv \left[(-1)^m\left(1-pH_m\right)\left(1+pH_m\right)\right]^4 \equiv \left[(-1)^m\right]^4 \equiv 1 \pmod{p^2}.$$

The only other possibility is $\sum k_i = p-1$. Therefore,

$$\gamma(p) \equiv -3p+(3p+1)\sum_{\substack{k_1,k_2,k_3,k_4=0\\ \sum k_i = p-1}}^{m} f(p,k_1,k_2,k_3,k_4) \pmod{p^2}.$$

Noting that $H_{m+j}-H_j \in \mathbb{Z}_p$ for $0 \leqslant j \leqslant m$, we have

$$f(p,k_1,k_2,k_3,k_4) = \prod_{i=1}^{4}\binom{m}{k_i}\binom{m+k_i}{k_i}(-1)^{k_i}\left(1+2pk_i\left(H_{m+k_i}-H_{k_i}\right)\right)$$

$$\equiv \left[\prod_{i=1}^{4}\binom{m}{k_i}\binom{m+k_i}{k_i}\right]\left(1+2p\sum_{i=1}^{4}k_i\left(H_{m+k_i}-H_{k_i}\right)\right) \pmod{p^2},$$

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and so

$$\gamma(p) \equiv -3p + p \sum_{\substack{k_1,k_2,k_3,k_4=0 \\ \sum k_i = p-1}}^{m} g(p,k_1,k_2,k_3,k_4) + \sum_{\substack{k_1,k_2,k_3,k_4=0 \\ \sum k_i = p-1}}^{m} \prod_{i=1}^{4} \binom{m}{k_i}\binom{m+k_i}{k_i} \pmod{p^2}, \tag{4·16}$$

where, for brevity,

$$g(p,k_1,k_2,k_3,k_4) := \left[\prod_{i=1}^{4} \binom{m}{k_i}\binom{m+k_i}{k_i}\right]\left(3 + 2\sum_{i=1}^{4} k_i \left(H_{m+k_i} - H_{k_i}\right)\right).$$

We will now show that

$$\sum_{\substack{k_1,k_2,k_3,k_4=0 \\ \sum k_i = p-1}}^{m} g(p,k_1,k_2,k_3,k_4) \equiv 3 \pmod{p}. \tag{4·17}$$

Using (4·5) and (4·1), we note that, when $\sum k_i = p-1$,

$$\begin{aligned} g(p,k_1,k_2,k_3,k_4) &\equiv \left[\prod_{i=1}^{4} (-1)^{k_i} \left(\frac{(k_i+1)_m}{(m)!}\right)^2\right]\left(3 + 2\sum_{i=1}^{4} k_i \left(H_{m+k_i} - H_{k_i}\right)\right) \\ &\equiv \left[\prod_{i=1}^{4} (k_i+1)_m^2\right]\left(3 + 2\sum_{i=1}^{4} k_i \left(H_{m+k_i} - H_{k_i}\right)\right) \pmod{p}. \end{aligned} \tag{4·18}$$

Let us define

$$\begin{aligned} &g_1(p,k_1,k_2,k_3,k_4) \\ &:= \left[\prod_{i=1}^{4} (k_i+1)_m^2\right]\left(3 + 2\sum_{i=1}^{3} k_i \left(H_{m+k_i} - H_{k_i}\right) - 2(k_1+k_2+k_3)\left(H_{m+k_4} - H_{k_4}\right)\right) \end{aligned} \tag{4·19}$$

as well as

$$g_2(p,k_1,k_2,k_3,k_4) := \left[\prod_{i=1}^{4} (k_i+1)_m^2\right] 2(p-1)\left(H_{m+k_4} - H_{k_4}\right).$$

Then, using (4·18) and Lemma 4·3, we get that

$$\begin{aligned} &\sum_{\substack{k_1,k_2,k_3,k_4=0 \\ \sum k_i = p-1}}^{m} g(p,k_1,k_2,k_3,k_4) \\ &\quad\equiv \sum_{\substack{k_1,k_2,k_3,k_4=0 \\ \sum k_i = p-1}}^{m} g_1(p,k_1,k_2,k_3,k_4) + \sum_{\substack{k_1,k_2,k_3,k_4=0 \\ \sum k_i = p-1}}^{m} g_2(p,k_1,k_2,k_3,k_4) \\ &\quad\equiv \sum_{\substack{k_1,k_2,k_3,k_4=0 \\ \sum k_i = p-1}}^{m} g_1(p,k_1,k_2,k_3,k_4) \pmod{p}. \end{aligned}$$

If $m < k < p$, then $H_{m+k} - H_k \in \frac{1}{p}\mathbb{Z}_p$ and $(k+1)_m \in p\mathbb{Z}_p$. Therefore, to establish (4·17)

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it suffices to prove

$$\sum_{\substack{k_1,k_2,k_3,k_4=0\\ \sum k_i = p-1}}^{p-1} g_1(p,k_1,k_2,k_3,k_4) \equiv 3 \pmod{p}. \tag{4·20}$$

Let $k_4 := p-1-k_1-k_2-k_3$ and consider, for $1 \leqslant i \leqslant 3$,

$$\begin{aligned} P(k_i) &:= \frac{d}{dk_i}\left[k_i\,(k_i+1)_m^2\,(k_4+1)_m^2\right] = b_{i,0} + \sum_{t=1}^{4m} b_{i,t}k_i^t \\ &= k_i\,(k_i+1)_m^2\,\frac{d}{dk_i}\left[(k_4+1)_m^2\right] + (k_4+1)_m^2\,\frac{d}{dk_i}\left[k_i\,(k_i+1)_m^2\right]. \end{aligned}$$

Now,

$$\begin{aligned} \frac{d}{dk_i}\left[k_i\,(k_i+1)_m^2\right] &= (k_i+1)_m^2 + k_i\,\frac{d}{dk_i}\left[(k_i+1)_m^2\right] \\ &= (k_i+1)_m^2 + k_i\left[2\,(k_i+1)_m\,\frac{d}{dk_i}(k_i+1)_m\right] \\ &= (k_i+1)_m^2 + k_i\left[2\,(k_i+1)_m\sum_{s=1}^{m}\prod_{\substack{r=1\\ r\neq s}}^{m}(k_i+r)\right] \\ &= (k_i+1)_m^2\left[1+2k_i\sum_{s=1}^{m}\frac{1}{(k_i+s)}\right] \\ &= (k_i+1)_m^2\left[1+2k_i\left(H_{m+k_i}-H_{k_i}\right)\right], \end{aligned}$$

and, similarly,

$$\begin{aligned} \frac{d}{dk_i}\left[(k_4+1)_m^2\right] &= 2\,(k_4+1)_m\,\frac{d}{dk_i}\left[(k_4+1)_m\right] \\ &= 2\,(k_4+1)_m\,\frac{d}{dk_i}\left[(p-1-k_1-k_2-k_3+1)_m\right] \\ &= -2\,(k_4+1)_m\sum_{s=1}^{m}\prod_{\substack{r=1\\ r\neq s}}^{m}(p-1-k_1-k_2-k_3+r) \\ &= -2(k_4+1)_m^2\left(H_{m+k_4}-H_{k_4}\right). \end{aligned}$$

So,

$$P(k_i) = (k_i+1)_m^2\,(k_4+1)_m^2\left[1+2k_i\left(H_{m+k_i}-H_{k_i}\right)-2k_i\left(H_{m+k_4}-H_{k_4}\right)\right]. \tag{4·21}$$

Noting (4·7), we see that

$$\sum_{k_1=0}^{p-1} P(k_i) = p\,b_{i,0} + \sum_{k_1=1}^{p-1}\sum_{t=1}^{4m} b_{i,t}k_i^t \equiv \sum_{t=1}^{4m} b_{i,t}\sum_{k_1=1}^{p-1} {k_i}^t \equiv -b_{i,p-1} - b_{i,2(p-1)} \pmod{p}.$$

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By definition of $P(k_i)$, we have that

$$(k_i+1)_m^2\,(k_4+1)_m^2 = b_{i,0} + \sum_{t=1}^{4m} \frac{b_{i,t}}{t+1} k_i^t\,,$$

which is monic with integer coefficients. Thus, $p \mid b_{i,p-1}$ and $b_{i,2(p-1)} = 2p-1$. Therefore,

$$\sum_{k_i=0}^{p-1} P(k_i) \equiv -b_{i,p-1} - b_{i,2(p-1)} \equiv 1 \pmod{p}. \tag{4·22}$$

Considering (4·19), accounting for (4·21) and (4·22), and applying Lemma 4·2, we get that

$$\begin{aligned}\sum_{\substack{k_1,k_2,k_3,k_4=0\\ \sum k_i = p-1}}^{p-1} g_1(p,k_1,k_2,k_3,k_4) &= \sum_{k_1,k_2,k_3=0}^{p-1} \sum_{i=1}^{3} \left[\prod_{\substack{j=1\\ j\neq i}}^{3} (k_j+1)_m^2\right] P(k_i)\\ &= \sum_{i=1}^{3} \sum_{\substack{k_j=0\\ j\neq i}}^{p-1} \left[\prod_{\substack{j=1\\ j\neq i}}^{3} (k_j+1)_m^2\right] \sum_{k_i=0}^{p-1} P(k_i)\\ &\equiv \sum_{i=1}^{3} \sum_{\substack{k_j=0\\ j\neq i}}^{p-1} \left[\prod_{\substack{j=1\\ j\neq i}}^{3} (k_j+1)_m^2\right] \equiv \sum_{i=1}^{3} 1 = 3 \pmod{p}.\end{aligned}$$

This establishes (4·20), which in turn establishes (4·17). Now, accounting for (4·17) in (4·16), we see that

$$\gamma(p) \equiv \sum_{\substack{k_1,k_2,k_3,k_4=0\\ \sum k_i = p-1}}^{\frac{p-1}{2}} \prod_{i=1}^{4} \binom{\frac{p-1}{2}}{k_i}\binom{\frac{p-1}{2}+k_i}{k_i} \pmod{p^2}.$$

Applying Lemma 4·4 completes the proof.

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REFERENCES

[**1**] S. AHLGREN. Gaussian hypergeometric series and combinatorial congruences. In *Symbolic computation, number theory, special functions, physics and combinatorics*. Dev. Math. **4** (Kluwer Academic Publisher, Dordrecht, 2001), pp.1–12.

[**2**] S. AHLGREN. The points of a certain fivefold over finite fields and the twelfth power of the eta function. *Finite Fields Appl.* **8** (2002), 18–33.

[**3**] S. AHLGREN and K. ONO. A Gaussian hypergeometric series evaluation and Apéry number congruences. *J. Reine Angew. Math.* **518** (2000), 187–212.

https://doi.org/10.1017/S0305004118000774 Published online by Cambridge University Press

[**4**] T. AMDEBERHAN and R. TAURASO. Supercongruences for the Almkvist–Zudilin numbers. *Acta Arith.* **173** (2016), 255–268.
[**5**] G. ALMKVIST, C. VAN ENCKEVORT, D. VAN STRATEN and W. ZUDILIN. Tables of Calabi–Yau equations. Preprint (2010), arXiv:math/0507430v2
[**6**] B. ASPVALL and F. LIANG. The dinner table problem. Technical Report STAN-CS-80-829, Computer Science Department, Stanford University, Stanford, California, 1980.
[**7**] F. BEUKERS. A note on the irrationality of $\zeta(2)$ and $\zeta(3)$. *Bull. London Math. Soc.* **11** (1979), 268–272.
[**8**] F. BEUKERS. Some congruences for the Apéry numbers. *J. Number Theory* **21** (1985), 141–155.
[**9**] F. BEUKERS. Another congruence for the Apéry numbers. *J. Number Theory* **25** (1987), 201–210.
[**10**] C. BOGNER and F. BROWN. Feynman integrals and iterated integrals on moduli spaces of curves of genus zero. *Commun. Number Theory Phys.* **9** (2015), 189–238.
[**11**] J. BROEDEL, O. SCHLOTTERER and S. STIEBERGER. Polylogarithms, multiple zeta values and superstring amplitudes. *Fortschr. Phys.* **61** (2013), 812–870.
[**12**] F. BROWN. Multiple zeta values and periods of moduli spaces $\overline{\mathcal{M}}_{0,n}$. *Ann. Sci. Éc. Norm. Supér* (4) **42** (2009), 371–489.
[**13**] F. BROWN. Irrationality proofs for zeta values, moduli spaces and dinner parties. *Mosc. J. Comb. Number Theory* **6** (2016), 102–165.
[**14**] F. BROWN, S. CARR and L. SCHNEPS. The algebra of cell-zeta values. *Compos. Math.* **146** (2010), 731–771.
[**15**] H. H. CHAN, S. COOPER and F. SICA. Congruences satisfied by Apéry-like numbers. *Int. J. Number Theory* **6** (2010), 89–97.
[**16**] S. COOPER. Sporadic sequences, modular forms and new series for $1/\pi$. *Ramanujan J.* **29** (2012), 163–183.
[**17**] M. COSTER. Supercongruences. PhD. thesis, Universiteit Leiden (1988).
[**18**] C. DUPONT. Odd zeta motive and linear forms in odd zeta values. With a joint appendix with Don Zagier. *Compos. Math.* **154** (2018), 342–379.
[**19**] S. FRECHETTE, K. ONO and M. PAPANIKOLAS. Gaussian hypergeometric functions and traces of Hecke operators. *Int. Math. Res. Notices* 2004, 3233–3262.
[**20**] I. GESSEL. Some congruences for Apéry numbers. *J. Number Theory* **14** (1982), 362–368.
[**21**] V. V. GOLYSHEV and D. ZAGIER. Proof of the gamma conjecture for Fano 3-folds of Picard rank 1. *Izv. Math.* **80** (2016), 24–49.
[**22**] A. B. GONCHAROV and Y. I. MANIN. Multiple ζ-motives and moduli spaces $\overline{\mathcal{M}}_{0,n}$. *Compos. Math.* **140** (2004), 1–14.
[**23**] J. GREENE. Hypergeometric functions over finite fields. *Trans. Amer. Math. Soc.* **301** (1987), 77–101.
[**24**] G. H. HARDY and E. M. WRIGHT. *An introduction to the theory of numbers*. Fifth edition. (The Clarendon Press, Oxford University Press, New York, 1979).
[**25**] G. KALITA and A. CHETRY. Congruences for generalised Apéry numbers and Gaussian hypergeometric series. *Res. Number Theory* **3** (2017), Art. 5, 15 pp.
[**26**] M. KOIKE. Orthogonal matrices obtained from hypergeometric series over finite fields and elliptic curves over finite fields. *Hiroshima Math. J.* **25** (1995), 43–52.
[**27**] C. KOUTSCHAN. Advanced Applications of the Holonomic Systems Approach. PhD. thesis. RISC, Johannes Kepler University, Linz, Austria (2009).
[**28**] P. LAIREZ. Computing periods of rational integrals. *Math. Comp.* **85** (2016), 1719–1752.
[**29**] P. LOH and R. RHODES. p-adic and combinatorial properties of modular form coefficients. *Int. J. Number Theory* **2** (2006), 305–328.
[**30**] K. ONO. Values of Gaussian hypergeometric series. *Trans. Amer. Math. Soc.* **350** (1998), 1205–1223.
[**31**] R. OSBURN and B. SAHU. Congruences via modular forms. *Proc. Amer. Math. Soc.* **139** (2011), 2375–2381.
[**32**] R. OSBURN AND B. SAHU. Supercongruences for Apéry-like numbers. *Adv. in Appl. Math.* **47** (2011), 631–638.
[**33**] R. OSBURN and B. SAHU. A supercongruence for generalised Domb numbers. *Funct. Approx. Comment. Math.* **48** (2013), 29–36.
[**34**] R. OSBURN, B. SAHU and A. STRAUB. Supercongruences for sporadic sequences. *Proc. Edinb. Math. Soc.* (2) **59** (2016), 503–518.
[**35**] R. OSBURN and C. SCHNEIDER. Gaussian hypergeometric series and supercongruences. *Math. Comp.* **78** (2009), 275–292.
[**36**] R. OSBURN and A. STRAUB. Interpolated sequences and critical L-values of modular forms. Preprint (2018), arXiv:1806.05207

https://doi.org/10.1017/S0305004118000774 Published online by Cambridge University Press

[**37**] E. PANZER. Algorithms for the symbolic integration of hyperlogarithms with applications to Feynman integrals. *Comput. Phys. Commun.* **188** (2015), 148–166.
[**38**] P. POULET. Permutations. *L'Intermédiaire des Mathématiciens* **26** (1919), 117–121.
[**39**] K. RIBET. Galois representations attached to eigenforms with Nebentypus. In *Modular functions of one variable, V*, Lecture Notes in Math. vol. 601 (Springer, 1977), pp. 17–51.
[**40**] D.P. ROBERTS, F. RODRIQUEZ–VILLEGAS and M. WATKINS. Hypergeometric motives. "Preprint" (2017).
[**41**] O. SCHLOTTERER and S. STIEBERGER. Motivic multiple zeta values and superstring amplitudes. *J. Phys. A* **46** (2013), 475401, 37 pp.
[**42**] J. STIENSTRA and F. BEUKERS. On the Picard–Fuchs equation and the formal Brauer group of certain elliptic $K3$-surfaces. *Math. Ann.* **271** (1985), 269–304.
[**43**] A. STRAUB. Multivariate Apéry numbers and supercongruences of rational functions. *Algebra Number Theory* **8** (2014), 1985–2008.

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